

WHAT IS CLAIMED IS:

1. A method for determining an ion concentration in solution of each of at least two ions capable of undergoing transport in a cement-based material under a chemical attack and a solid phase profile for at least one component of said cement-based material, said cement-based material having a solid skeleton and pores, said pores being at least one of liquid-filled and vapor-filled, a porosity of said cement-based material being provided, the method comprising the steps of:

determining a first concentration for each said at least two ions and an electrical potential profile using a transport algorithm, wherein the transport algorithm is a function of a diffusion of said at least two ions, of an adsorption of said at least two ions, of an electrical coupling between said at least two ions and a chemical activity of said at least two ions and wherein an ionic solution of said material is not in equilibrium with various solid phases of an hydrated paste of said cement-based material;

calculating a corrected concentration for each of said at least two ions and a first solid phase profile for each said at least one component using a chemical reactions algorithm, wherein at least one of a dissolution and a precipitation reactions is accounted for in order to maintain an equilibrium between said ionic solution and said various solid phases of said hydrated paste;

calculating a changed transport properties profile to take into account an effect of said chemical reactions on said porosity of said material; and

determining an ion concentration for each of said at least two ions and a solid phase profile for each of said at least one component using said changed transport properties profile, said corrected concentration and said first solid phase profile, wherein effects of said chemical reactions on an ionic transport are taken into account by correcting material transport properties

whereby said ion concentration for each said at least two ions and said solid phase profile for each said at least one component in said cement-based material can be used to evaluate a degradation of said cement-based material.

2. A method as claimed in claim 1, wherein said step of calculating a first concentration comprises solving a set of equations.

3. A method as claimed in claim 2, wherein said set of equations is solved using a finite elements method.

4. A method as claimed in claim 1, further comprising a step of providing input data, said input data comprising a porosity, a temperature, ionic pore solution concentrations, an amount of each solid phase, a diffusion coefficient for each ionic species, a water diffusivity and an initial water content.

5. A method as claimed in claim 4, wherein said input data further comprises a finite element mesh and boundary conditions.

6. A method as claimed in claim 5, wherein said chemical reactions algorithm is performed on each node of said finite element mesh.

7. A method as claimed in claim 4, wherein said input data further comprises a number of time steps and a length of said time steps.

8. A method as claimed in claim 7, further comprising a step of determining a profile of said ion concentration by repeating said steps of determining a first concentration, calculating a corrected concentration, calculating a changed transport properties profile and determining an ion concentration and solid phase profile for each of said time steps.

9. A method as claimed in claim 1, further comprising a step of generating an indication of said ion concentration and an indication of said solid phase profile.

10. A method as claimed in claim 1, further comprising a step of determining a porosity profile using said solid phase profile, said ion concentration profiles and said electrical potential profile.

11. A method as claimed in claim 10, further comprising a step of generating an indication of said porosity profile.

12. A method as claimed in claim 1, wherein said components are at least one of C-S-H, Gypsum, Portlandite, Mirabilite, Ettringite and Hydrogarnet.

13. A method as claimed in claim 1, wherein said ions are at least one of OH^- , Na^+ , K^+ , SO_4^{2-} , Ca^{2+} and $\text{Al}(\text{OH})_4^-$.

14. A method as claimed in claim 1, wherein said step of determining a first concentration is carried out before said step of calculating a corrected concentration.

15. A method as claimed in claim 1, wherein said transport algorithm is further a function of a capillary suction, said capillary suction arising when said material is exposed to a gradient of relative humidity, said transport algorithm thereby determining a water content profile.

16. A method as claimed in claim 15, further comprising a step of providing input data, said input data comprising a porosity, a temperature, ionic pore solution concentrations, an amount of each solid phase, a diffusion coefficient for each ionic species, a water diffusivity and an initial water content.

17. A method as claimed in claim 16, wherein said input data further comprises a number of time steps and a length of said time steps.

18. A method as claimed in claim 17, further comprising a step of determining a profile of said ion concentration by repeating said steps of determining a first concentration, calculating a corrected concentration, calculating a changed transport properties profile and determining an ion concentration and solid phase profile for each of said time steps.

19. A method for determining a diffusion coefficient for each of at least two ions capable of undergoing transport in a cement-based material, said cement-based material having a solid skeleton and pores, said pores being at least one of liquid-filled and vapor-filled, a porosity of said cement-based material being provided, the method comprising the steps of:

- determining a concentration for each said at least two ions and an electrical potential profile using a transport algorithm, wherein the transport algorithm is a function of a diffusion of said at least two ions, of an electrical coupling between said at least two ions and a chemical activity of each said at least two ions; and

- determining a diffusion coefficient for each of at least two ions using said concentration and said electrical potential profile.

20. A method as claimed in claim 19, further comprising:

- providing input data, said input data comprising a set of tortuosity parameters and a measured electrical current for said material, and

- determining a diffusion coefficient for each of said ions by

- calculating a set of electrical currents each electrical current corresponding to one of said tortuosity parameter in said set of tortuosity parameters using said concentration, said electrical potential and each one of said tortuosity parameter in said set of tortuosity parameters;

- choosing an electrical current from said set with a value closest to said measured electrical current;

- determining a matching tortuosity parameter corresponding to said chosen electrical current; and

determining said diffusion coefficient for each of said ions using said matching tortuosity.